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# Simulates the 15 day mouse exposure study
# Data collected during and after exposure on 1st day
# and at end of exposure on day 5 and 15 (1 day nose-only)
#Uses Table 3 metabolism rates

#set the working directory to where you downloaded the scripts
setwd(dirname(parent.frame(2)$ofile))

# load libraries needed to run scenario
library(deSolve)

# Model path and name
mName <- "chloroprene.model"

#load model inits file for the ode solver
source(paste0(mName, "_inits.R"))

#load the states files
#source(paste0(mPath, "states.R"))

#load the model dll
dyn.load(paste0(mName, .Platform$dynlib.ext))

#Scenario specific values
tstart <- 0.0
tstop <- 336
times <- seq(tstart, tstop , by=0.05)

# Physiolgical parameters path

#load the parameters
source('./params/Mouse.R')
source('./states.R')

# timing variables for forcing functions
dstart <- tstart
dlength <- 6.0      #hours per day to expose
ddaysperwk <- 5    #days of week to expose
dexpend <- 19      #days of exposure
parms["TSTOP"] <- tstop

# Source forcing functions
# this loads the function forcing() in the namespace
source("forfunc.R")

#*****
#*****
#Simulation specific metabolism parameters
parms["VMAXC"] <- 7.95    # Liver
parms["KM"] <- 0.041

parms["VMAXCLU"] <- 0.18  # Lung
parms["KMLU"] <- 0.26

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parms["KFLUC"] <- 0.0

parms["VMAXCKid"] <- 0.00 # Kidney
parms["KMKD"] <- 1.0
parms["KFKIC"] <- 0.079
#*****
#*****

bout = 0
pout = 0
clouta = 0
c2outa = 0
cloutb = 0
c2outb = 0
cloutc = 0
c2outc = 0

# Run base model

for(i in 1:1){

  parms["CONC"]<- 12.8
  out <- ode(Y, times, func = "derivs", parms = parms, method="vode",
    atol=1.0e-10, rtol=1.0e-8,
    dllname = mName, initforc="initforc", forcings=forcings,
    initfunc = "initmod", nout = length(Outputs),
    outnames = Outputs)

  clouta[[i]] <- out[tstop/0.05+1, 23]

#Scenario Specific Exposure
parms["CONC"]<- 32.0

# Run ODE

  out <- ode(Y, times, func = "derivs", parms = parms, method="vode",
    atol=1.0e-10, rtol=1.0e-8,
    dllname = mName, initforc="initforc", forcings=forcings,
    initfunc = "initmod", nout = length(Outputs),
    outnames = Outputs)

  cloutb[[i]] <- out[tstop/0.05+1, 23]

#Scenario Specific Exposure
parms["CONC"]<- 80.0

# Run ODE

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    out <- ode(Y, times, func = "derivs", parms = parms, method="vode",
              atol=1.0e-10, rtol=1.0e-8,
              dllname = mName, initforc="initforc", forcings=forcings,
              initfunc = "initmod", nout = length(Outputs),
              outnames = Outputs)
    cloutc[[i]] <- out[tstop/0.05+1, 23]

}

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clouta <- data.frame(clouta)
cloutb <- data.frame(cloutb)
cloutc <- data.frame(cloutc)

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bout <- cbind(clouta,cloutb,cloutc)
colnames(bout)<- c("12.8", "32.0","80.0")

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pname <- c("BW",
           "QPC",
           "QCC",
           "QLC",
           "QFC",
           "QSC",
           "QKC",
           "VLC",
           "VLUC",
           "VFC",
           "VRC",
           "VSC",
           "VKC",
           "PL",
           "PLU",
           "PF",
           "PS",
           "PR",
           "PB",
           "PK",
           "VMAXC",
           "KM",
           "VMAXCLU",
           "KMLU",
           "KFKIC" )

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pval <- c(0.03 ,
          29.1 ,
          20.1 ,
          0.161 ,
          0.07 ,
          0.159 ,
          0.09 ,
          )

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0.055 ,
0.0073 ,
0.1 ,
0.08098,
0.384 ,
0.0167 ,
1.26 ,
2.38 ,
17.35 ,
0.59 ,
1.76 ,
7.8 ,
1.76 ,
7.95 ,
0.041 ,
0.18 ,
0.26 ,
0.079
)

print(system.time(
  for(i in 1:length(pval)){
    source('./params/Mouse.R',local=TRUE)

    #*****
    #*****
    #Simulation specific metabolism parameters
    parms["VMAXC"] <- 7.95 # Liver
    parms["KM"] <- 0.041

    parms["VMAXCLU"] <- 0.18 # Lung
    parms["KMLU"] <- 0.26
    parms["KFLUC"] <- 0.0

    parms["VMAXCKid"] <- 0.00 # Kidney
    parms["KMKD"] <- 1.0
    parms["KFKIC"] <- 0.079
    #*****
    #*****
    parms["TSTOP"] <- tstop

    pnameb <- pname[i]
    pvalb <- pval[i]
    parms[pnameb] <- pvalb*1.01

    parms["CONC"]<- 12.8
    out <- ode(Y, times, func = "derivs", parms = parms, method="vode",
      atol=1.0e-10, rtol=1.0e-8,
      dllname = mName, initforc="initforc", forcings=forcings,
      initfunc = "initmod", nout = length(Outputs),

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        outnames = Outputs)

c2outa[[i]] <- out[tstop/0.05+1, 23]

#Scenario Specific Exposure
parms["CONC"]<- 32.0

# Run ODE

out <- ode(Y, times, func = "derivs", parms = parms, method="vode",
          atol=1.0e-10, rtol=1.0e-8,
          dllname = mName, initforc="initforc", forcings=forcings,
          initfunc = "initmod", nout = length(Outputs),
          outnames = Outputs)

c2outb[[i]] <- out[tstop/0.05+1, 23]

#Scenario Specific Exposure
parms["CONC"]<- 80.0

# Run ODE

out <- ode(Y, times, func = "derivs", parms = parms, method="vode",
          atol=1.0e-10, rtol=1.0e-8,
          dllname = mName, initforc="initforc", forcings=forcings,
          initfunc = "initmod", nout = length(Outputs),
          outnames = Outputs)
c2outc[[i]] <- out[tstop/0.05+1, 23]

    }
  ))

c2outa <- data.frame(c2outa)
c2outb <- data.frame(c2outb)
c2outc <- data.frame(c2outc)

pout <- cbind(c2outa,c2outb,c2outc)
colnames(pout)<- c("12.8", "32.0","80.0")

allout = 0

allout <- data.frame(rbind(bout,pout))
colnames(allout)<- c("12.8ppm", "32.0ppm", "80.0ppm")

#unload the model dll
dyn.unload(paste0(mName, .Platform$dynlib.ext))

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write.csv(allout, file='mouseinvivometric_sa.csv')
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